ECE 371
Materials and Devices

09/03/19 - Lecture 4

Schrodinger’s Equation: Meaning of the Wave Function and Free Electron Solution

General Information

- Homework #1 due before class today
- Homework #2 assigned and due Thursday September 12^{th}
- Link to download Crystal Viewer (http://crystalmaker.com/crystalviewer/index.html) added to the website in Articles, Videos, and Additional Notes folder. See next few slides for examples of software capabilities.
- Reading for next time: 2.3.2-2.3.3

Wave Function

- The temporal and spatial evolution of a particle (e.g., electron) with one degree of freedom is given by $\psi(x, t)$
- $\psi(x, t)$ can be complex
- $\psi(x, t) \cdot \psi^*(x, t)$ is related to the probability of finding the particle within the interval $x + dx$
- The shape of the wave function is influenced by the potential energy landscape

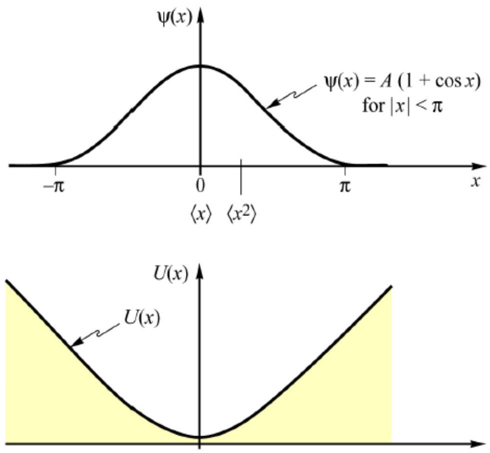


Fig. 2.1. Example for a one-dimensional wave function $\psi(x)$. Also shown is a corresponding potential function, $U(x)$. This potential function provides a driving force towards $x = 0$, that is towards minimum energy.

Schubert, "Physical Foundations of Solid State Devices"

Schrodinger's Wave Equation

- The Schrodinger equation (SE) describes the spatial and temporal evolution of the wave function for a given potential energy landscape and set of boundary conditions

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t)=j\hbar\frac{\partial\psi(x,t)}{\partial t}}$$

related to kinetic energy | related to potential energy | related to total energy

- $V(x)$ is the potential energy, m is the mass of the particle, and $j=\sqrt{-1}$

for crystals – use "effective mass"

- SE is a basic postulate of quantum mechanics but can be derived
- SE can be used to describe the behavior of electrons in a crystal

Time-Dependent and Time-Independent Parts of SE

- The separation of variables technique can be used to deconstruct the SE into time-dependent and time-independent parts
- We assume that the wave function can be represented as the product of a time-independent function and a time-dependent function (i.e., $\psi(x,t) = \psi(x)\phi(t)$)

Focus on Solutions to potential energy (i.e. electron in well)

Time-dependent solution can be obtained quickly:

$$\boxed{\phi(t) = e^{-j\left(\frac{E}{\hbar}\right)t} = e^{-j\omega t}}$$

Sinusoidal variation with time

E is the total energy of the particle

$E = \hbar\omega$

Time-independent part of the equation:

$$\boxed{\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\big(E - V(x)\big)\psi(x) = 0}$$

potential

Nature of the solution for $\psi(x)$ depends upon the potential V(x) and the boundary conditions

Types of solutions will be $\psi(x) =$ sins & cosines

*see in-class derivation

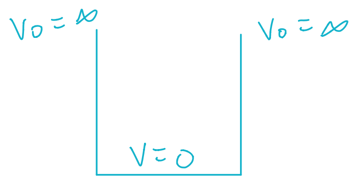
Solve 3 different potentials:

(1) Free electron (zero potential ($V_x = 0$))

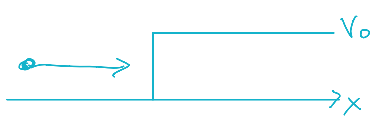
(can treat crystals as almost free electron)

(2) Infinite potential well

($V = 0$ inside ∞ outside)



(3) Potential Step

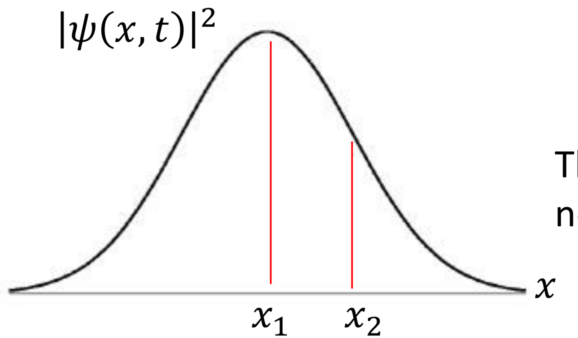


Physical Meaning of the Wave Function

- Use $\psi(x,t)$ to describe the behavior of electrons in crystals
- Wave function is complex so cannot itself represent a physical quantity
- Instead we define a probability density function that describes the probability of finding the electron between x and $x + dx$

$$\boxed{|\psi(x,t)|^2 = \psi(x)\psi^*(x) = |\psi(x)|^2}$$

- Probability density function of a variable describes the relative likelihood of the variable to take on a given value



Probability that the electron is between x_1 and x_2 is

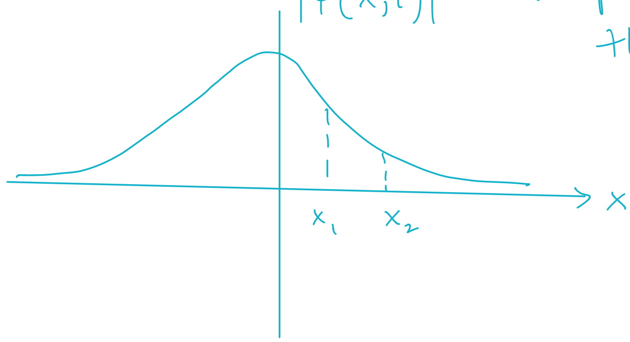
$$\boxed{\int_{x_1}^{x_2} |\psi(x)|^2 \, dx}$$

The electron must be somewhere so we can also normalize the wave function

$$\boxed{\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1}$$

$$\Psi(x,t) = \Psi(x)\,\phi(t) = \Psi(x)\,e^{-j\omega t}$$

$|\Psi(x,t)|^2 \rightarrow$ probability of finding the particle



$$\int_{x_1}^{x_2} |\Psi(x)|^2 \, dx$$

given potential $\rightarrow$ solve for Ψ and boundary conditions

Electron in Free Space

completely kinetic

When V(x) = 0 we have a free electron and the TISE becomes:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

Time independent Schrod. eq.

wave number:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

The general solution is two travelling waves:

$$\psi(x,t) = A\,exp[j(kx - \omega t)] + B\,exp[-j(kx + \omega t)]$$

For a travelling wave in the +x direction we have:

$$\psi(x,t) = A\,exp[j(kx - \omega t)]$$

particle only has kinetic energy

- The probability density function is a constant (AA^*)
- Particle can be found anywhere since the momentum is well defined
- Note that the plane wave solution cannot be normalized (but a superposition of plane waves can be – wave packet)

$$\underset{1\,=\,a}{\frac{d^2\psi(x)}{dx^2}} + \overset{c}{\boxed{\frac{2mE}{\hbar^2}}}\psi(x) = 0$$

linear
2^{nd} order
Homogeneous

$$ay'' + by' + cy = 0$$

$$\downarrow$$

$$r^2 + r + 0 = 0$$

$$\downarrow$$

$$r^2 + \frac{2mE}{\hbar^2} r = 0$$

$$r = \pm\sqrt{\frac{-2mE}{\hbar^2}} = \pm j\sqrt{\frac{-2mE}{\hbar^2}}$$

Soln has form:

$$y = c_1 e^{r_1 x} + c_2 e^{r_2 x}$$

$$\downarrow$$

$$\psi(x) = A e^{j\sqrt{\frac{2mE}{\hbar^2}}\,x} + B e^{-j\sqrt{\frac{2mE}{\hbar^2}}\,x}$$

↑ wave #

K (inversly proportional to wave length)

$$\psi(x) = A e^{jkx} + B e^{-jkx}$$

Adding back the time component:

$$\phi(t) = e^{-j\omega t}$$

$$\psi(x,t) = A\, exp[j(kx - \omega t)] + B\, exp[-j(kx + \omega t)]$$

$$\psi(x,t) = A e^{j(kx-\omega t)} + B e^{-j(kx+\omega t)}$$

What if:

Assume moving in pos x direction:

$B = 0$

$$\psi(x,t) = A e^{j(kx-\omega t)}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{p}{\hbar} = \frac{2\pi}{\lambda}$$

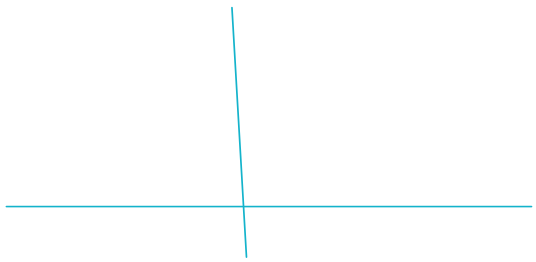
$p = \hbar k$ $\quad\quad$ $E = \hbar\omega = h\nu$

nu?

Probability Density

$$\Psi(x,t) \cdot \Psi^*(x,t) = A e^{j(kx-\omega t)} \cdot A e^{-j(kx-\omega t)}$$

$$= A \cdot A^* \longrightarrow \text{constant}$$



Potential Wells

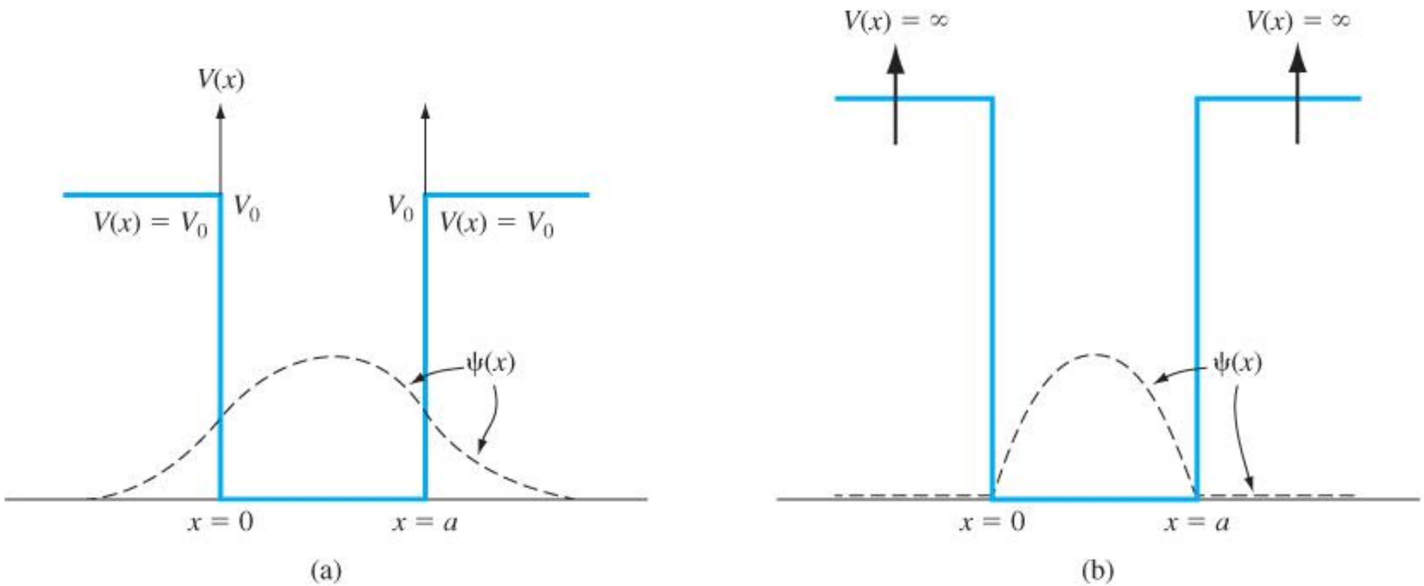


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

- Finite and infinite potential wells (bound particles)
- Potential height determines strength of confinement
- Solutions for $\psi(x)$ are sine and cosine functions for the infinite potential well